

## Electronic Supplementary Information

# **A Black Phosphorous/Ti<sub>3</sub>C<sub>2</sub> MXene Nanocomposite for Sodium-Ion Battery: Combined Experimental and Theoretical Study**

Anmin Liu <sup>a,\*</sup>, <sup>1</sup>, Huan Li <sup>b,1</sup>, Xuefeng Ren <sup>d</sup>, Yanan Yang <sup>a</sup>, Liguao Gao <sup>a</sup>, Meiqiang Fan <sup>c</sup>,  
and Tingli Ma <sup>b, c, \*</sup>

<sup>a</sup> State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology, China.

E-mail: [anmin0127@163.com](mailto:anmin0127@163.com), [liuanmin@dlut.edu.cn](mailto:liuanmin@dlut.edu.cn)

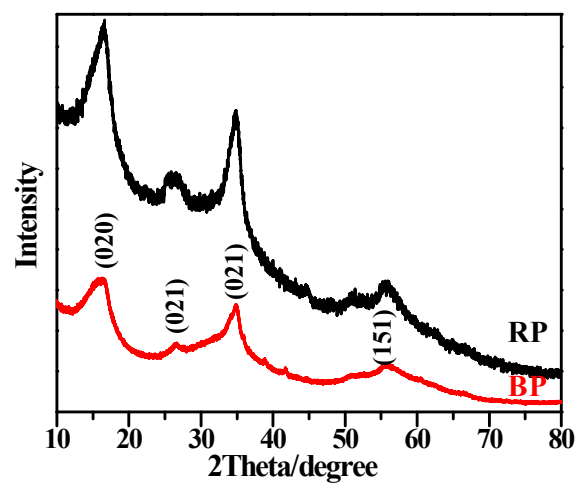
<sup>b</sup> Graduate School of Life Science and Systems Engineering, Kyushu Institute of Technology, 2-4 Hibikino, Wakamatsu, Kitakyushu, Fukuoka 808-0196, Japan.

E-mail: [tinglima@life.kyutech.ac.jp](mailto:tinglima@life.kyutech.ac.jp)

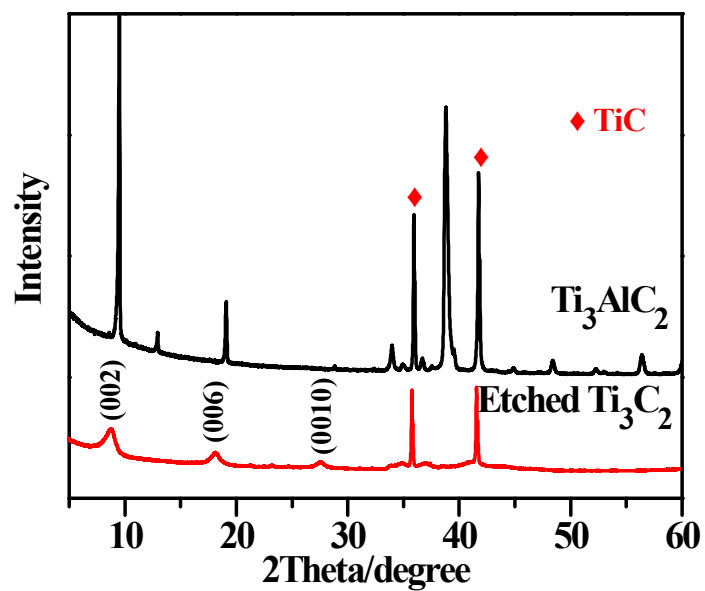
<sup>c</sup> Department of Materials Science and Engineering, China Jiliang University, Hangzhou, 310018, China.

<sup>d</sup> School of Food and Environment, Dalian University of Technology, Panjin, 124221, China.

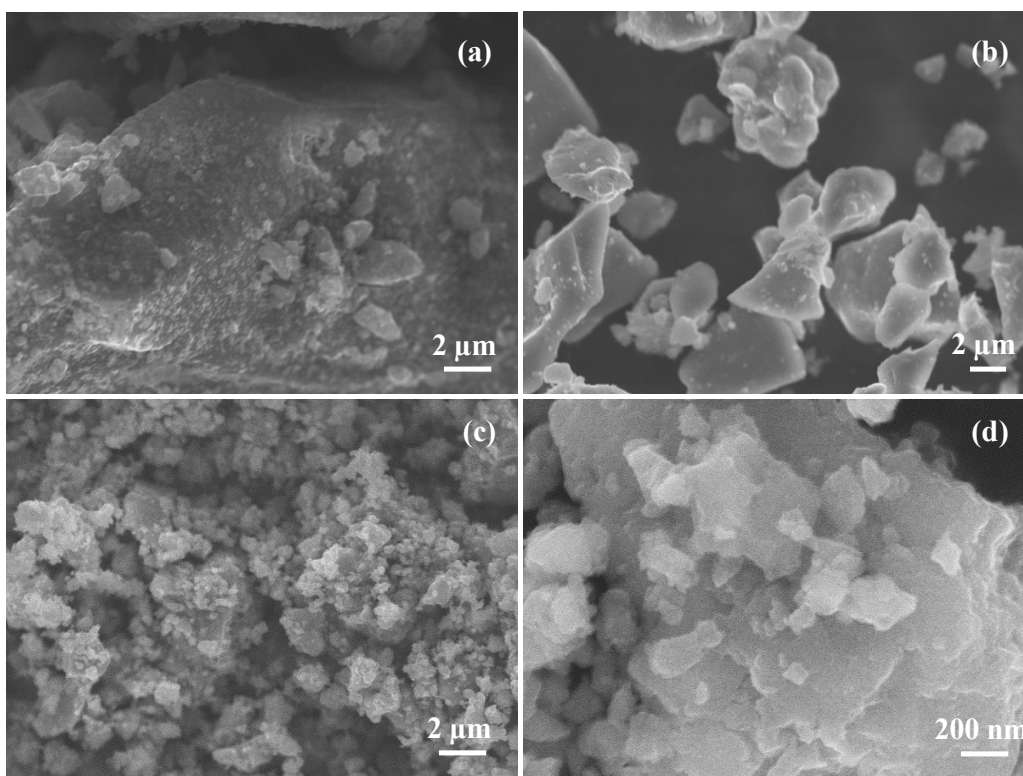
<sup>1</sup> These authors contributed equally to this work and should be considered co-first authors.



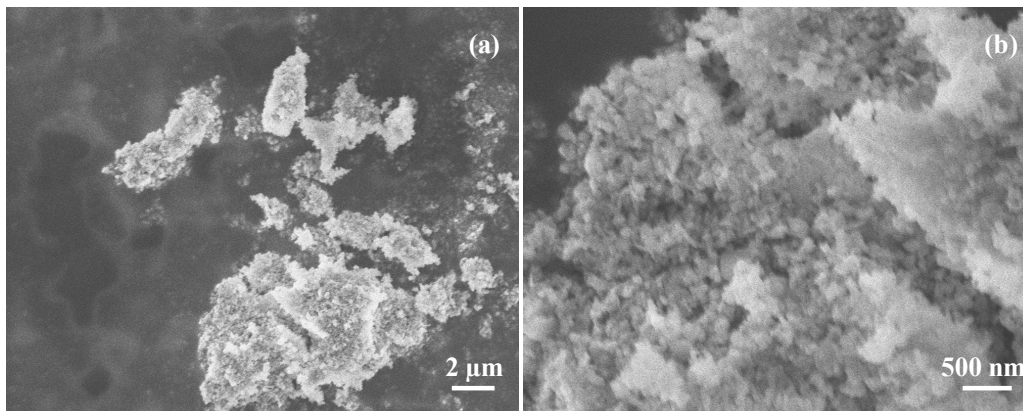
**Fig. S1** XRD patterns for RP and as-prepared BP after ball milling.



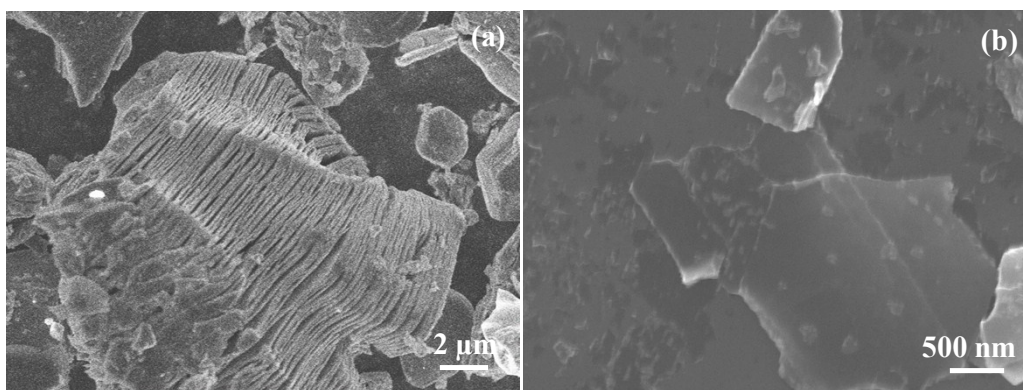
**Fig. S2** XRD patterns of MAX phase  $\text{Ti}_3\text{AlC}_2$  and products after etching by HF.



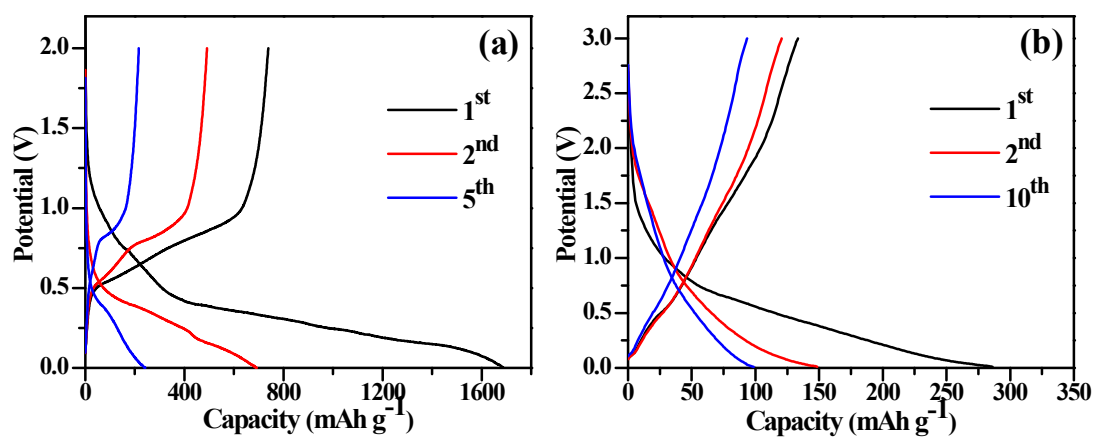
**Fig. S3** SEM images of the RP raw materials (a), RP after grind milling (b) and BP after ball milling (c-d).



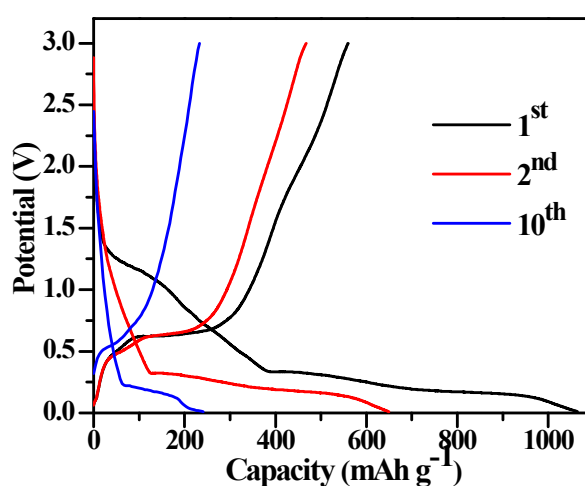
**Fig. S4** SEM images of BP after sonicating in DMF solution.



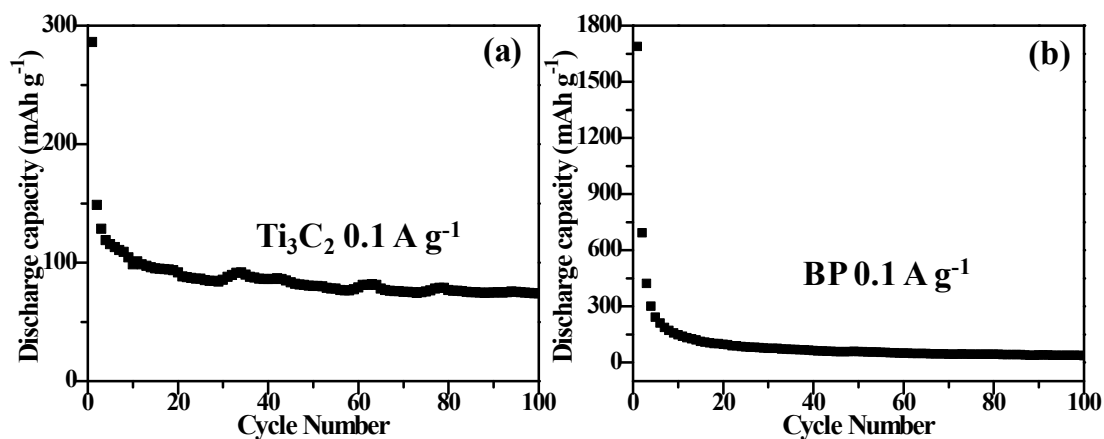
**Fig. S5** SEM images of bulk  $\text{Ti}_3\text{C}_2$  (a) and exfoliated  $\text{Ti}_3\text{C}_2$  nanoflakes in deionized water (b).



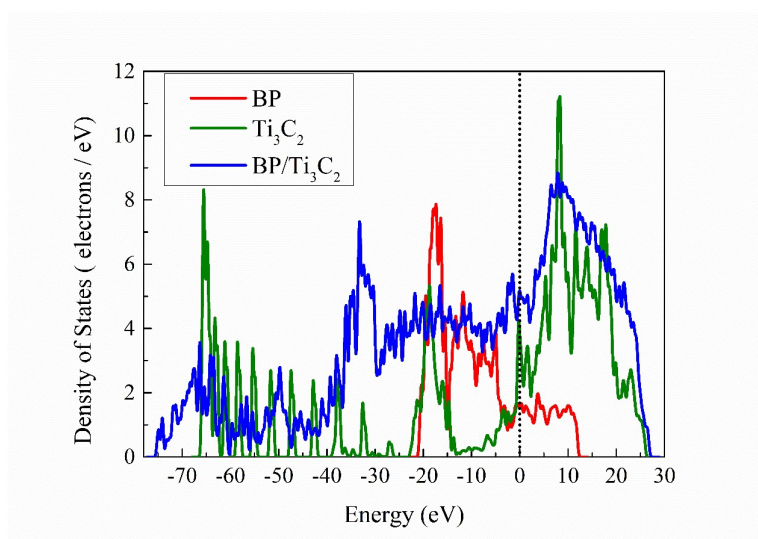
**Fig. S6** Charge-discharge profiles for the 1<sup>st</sup>, 2<sup>nd</sup> and 5<sup>th</sup> cycles of the BP electrode from 0.1 V-2.0 V (a) and the 1<sup>st</sup>, 2<sup>nd</sup> and 10<sup>th</sup> cycles for the  $\text{Ti}_3\text{C}_2$  electrode from 0.01 V-3.0 V at a current density of  $0.1 \text{ A g}^{-1}$ .



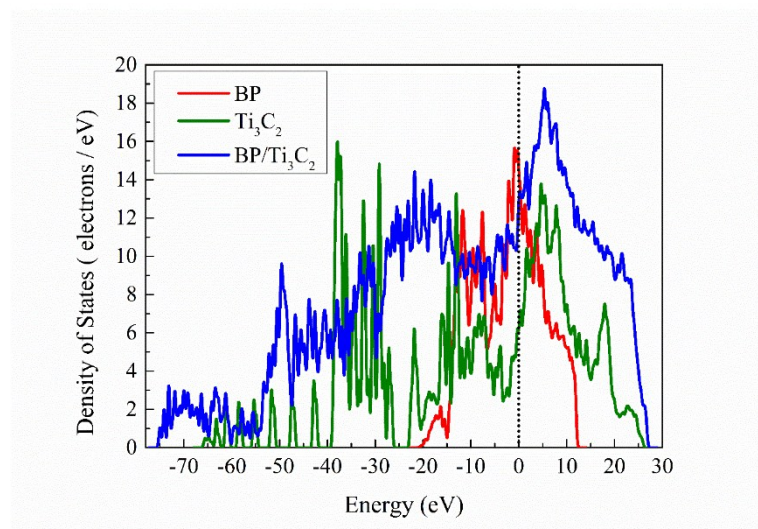
**Fig. S7** Charge-discharge profiles for the 1<sup>st</sup>, 2<sup>nd</sup> and 10<sup>th</sup> cycles of the BP/ $\text{Ti}_3\text{C}_2$  electrode from 0.01 V-3.0 V at a current density of  $0.5 \text{ A g}^{-1}$ .



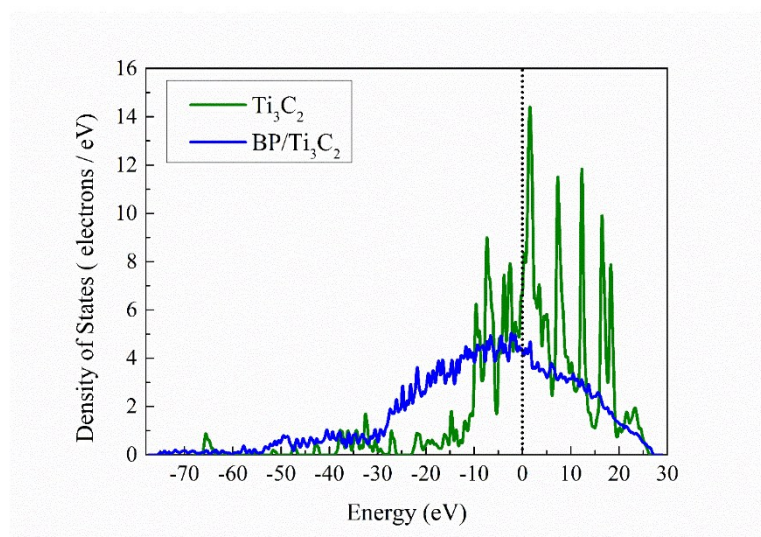
**Fig. S8** Cycling performance of the BP electrode (a) and  $\text{Ti}_3\text{C}_2$  electrode (b) at a current density of  $0.1 \text{ A g}^{-1}$ .



**Fig. S9** s orbit PDOS of BP,  $\text{Ti}_3\text{C}_2$ , and BP/ $\text{Ti}_3\text{C}_2$  composite.



**Fig. S10** p orbit PDOS of BP,  $\text{Ti}_3\text{C}_2$ , and BP/ $\text{Ti}_3\text{C}_2$  composite.



**Fig. S11** d orbit PDOS of BP,  $\text{Ti}_3\text{C}_2$ , and  $\text{BP}/\text{Ti}_3\text{C}_2$  composite.